AMENDMENTS TO AND LISTING OF CLAIMS

This listing of claims will replace all prior versions and listings of claims in this application.

1. (currently amended) A computer programmed to produce a three-dimensional representation of a molecule or molecular complex, wherein the molecule or molecular complex comprises a binding domain defined by ~~the~~ structure coordinates selected from the group consisting of (a) Arg 39, His 110, Ser 132, Thr136, Lys 254,Gly. 297, Lys 311, Thr 315, Arg337 and Asp339 according to Fig. 1; ~~or~~ (b) Ser 9,His 10, Arg39, Asp 54, Arg 107, His 110, Ser132, Ala133, Arg 134, Thr136, Arg 337 and Asp 339 according to Fig. 1, and ~~or where the~~ (c) a molecular complex or binding domain with ~~has~~ a root mean square deviation of conserved residue backbone atoms of less than2A when superimposed on the relevant backbone atoms described by the structure coordinates of said amino acids.

2. (currently amended) A computer programmed according to claim 1, wherein (a) further comprises the structure coordinates of (i) Arg 45, Gly109, Ala111, Ser131, Ala 133, Lys238, Asp 240, lie 250, Asn251, Ala 252, Phe 253, Phe 294, Gly 296, Met310, Ile 313, Pro 314, Ala 342, Ala 345, Ala 346 and Val 349 according to Fig. 1; and ~~or~~ (b) further comprises the structure coordinates of (ii) Arg 45, Met 49, Asp 80, Ser131, and Thr137 according to Fig.1, or where the molecular complex or binding domain has a root mean square deviation of conserved residue backbone atoms of less than2A when superimposed on the relevant backbone atoms described by the structure coordinates of said amino acids, or where the molecular complex or binding domain has conservative amino acid substitutions for those amino acids specified in (i) or (ii).

3. (currently amended) A computer programmed according to claims 1 or ~~claim~~ 2, wherein (a) further comprises the structure coordinates of Ser 338 according to Fig. 1, and ~~or~~ (b) further comprises the structure coordinates of Arg 48, Glu 336 and Ser 338 according to Fig.1.

4. (original) A computer according to any of claims 1 to 3, wherein the molecule is Chorismate Synthase.

5. (original) A computer according to any of claims 1 to 4, wherein the molecule is Chorismate Synthase from S. pneumoniae.

6. (currently amended) A method for identifying the potential of a chemical entity to associate with a Chorismate Synthase enzyme, comprising the steps of : (a) applying computational means to perform a fitting operation between the chemical entity and the Chorismate Synthase binding domain defined by the structure coordinates defined in any of claims 1 to 3; and (b) analysing the results of the fitting operation to quantify the association.

7. (original) A method according to claim 6, wherein the computational means is provided by a computer as defined in any of claims 1 to 5.

8. (currently amended) A method for identifying a potential inhibitor or agent that interacts with a Chorismate Synthase binding domain, comprising the steps of: (a) using the atomic coordinates defined in any of claims 1 to 3 to generate a three-dimensional structure of a molecule comprising a Chorismate Synthase binding domain; (b) employing the three-dimensional structure to design or select the inhibitor or agent; (c) synthesising the inhibitor or agent; and (d) contacting the inhibitor or agent with the Chorismate Synthase binding domain to determine the ability of the inhibitor or agent to interact with the domain.

9. (original) A crystal of the binding domain of Chorismate Synthase, wherein the binding domain has a three-dimensional structure characterised by the atomic structure coordinates of Fig. 1.

Applicants request that any questions concerning this matter be directed to the undersigned at (973) 775-8930.

Respectfully submitted,

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